

L13 ANSWER 17 OF 17 USPATFULL on STN

Full Text	References
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ACCESSION NUMBER: 89:6050 USPATFULL  
 TITLE: Pyridine-ethanolamine derivatives  
 INVENTOR(S): Alig, Leo, Kaiseraugst, Switzerland  
 Muller, Marcel, Frenkendorf, Switzerland  
 PATENT ASSIGNEE(S): Hoffmann-La Roche Inc., Nutley, NJ, United States (U.S. corporation)

	NUMBER	KIND	DATE
<u>PATENT INFORMATION:</u>	<u>US 4800206</u>		<u>19890124</u>
<u>APPLICATION INFO.:</u>	<u>US 1987-57150</u>		19870603 (7)

	NUMBER	DATE
<u>PRIORITY INFORMATION:</u>	<u>CH 1986-2608</u>	19860627
	<u>CH 1987-1186</u>	19870327

DOCUMENT TYPE: Utility  
 FILE SEGMENT: Granted  
 PRIMARY EXAMINER: Fan, Jane T.  
 LEGAL REPRESENTATIVE: Saxe, Jon S., Leon, Bernard S., Isgro, William G.  
 NUMBER OF CLAIMS: 21  
 EXEMPLARY CLAIM: 1  
 LINE COUNT: 879

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

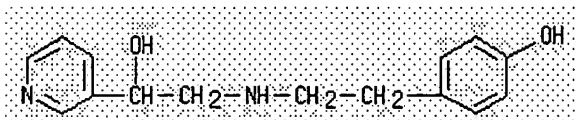
AB Pyridine-ethanolamines of the formula ##STR1## wherein n, X, Y, R<sup>1</sup>, R<sup>2</sup> and R<sup>3</sup> have the significances given in the description, their corresponding enantiomers, diastereomers, and racemates as well as the physiologically compatible salts thereof are described. The compounds of formula I have catabolic activity and can be used for the treatment of obesity and of diabetes mellitus or of conditions which are associated with an increased protein breakdown, or as feed additives for fattening animals. The compounds of formula I can be prepared by alkylating the primary or secondary amines corresponding to the secondary or tertiary amines of formula I.

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

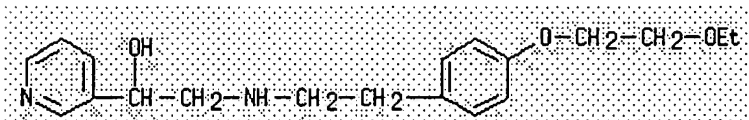
IT 115548-43-1P 115626-97-6P  
 (prepn. of, as remedy for obesity, diabetes mellitus, and elevated protein degrdn.)

RN 115548-43-1 USPATFULL

CN 3-Pyridinemethanol,  $\alpha$ -[[[2-(4-hydroxyphenyl)ethyl]amino]methyl]-  
 (9CI) (CA INDEX NAME)

RN 115626-97-6 USPATFULL

CN 3-Pyridinemethanol,  $\alpha$ -[[[2-[4-(2-ethoxyethoxy)phenyl]ethyl]amino]methyl]- (9CI) (CA INDEX NAME)



=>

L13 ANSWER 16 OF 17 USPATFULL on STN

Full Text	Bring References
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ACCESSION NUMBER: 89:102325 USPATFULL  
 TITLE: Synthetic flavonoids as inhibitors of leukotrienes and 5-lipoxygenase  
 INVENTOR(S): Wu, Edwin S., Rochester, NY, United States  
 Kover, Alexander, Rochester, NY, United States  
 PATENT ASSIGNEE(S): Fisons Corporation, Rochester, NY, United States (U.S. corporation)

	NUMBER	KIND	DATE
<b>PATENT INFORMATION:</b>	<b>US 4889941</b>		<b>19891226</b>
APPLICATION INFO.:	US 1987-129014		19871204 (7)
RELATED APPLN. INFO.:	Continuation-in-part of Ser. No. <u>US 1987-41817</u> , filed on 23 Apr 1987, now abandoned		
DOCUMENT TYPE:	Utility		
FILE SEGMENT:	Granted		
PRIMARY EXAMINER:	Chan, Nicky		
LEGAL REPRESENTATIVE:	Seidel, Gonda, Lavorgna & Monaco		
NUMBER OF CLAIMS:	1		
EXEMPLARY CLAIM:	1		
LINE COUNT:	699		

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

AB 7-[3-[(3,4-dihydroxyphenethyl)amino]-2-hydroxypropoxy]-flavone hydrobromide, and related flavonoids are disclosed to inhibit leukotrienes and 5-lipoxygenase; preferred compounds also inhibit rat anaphylaxis.

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

IT 119161-86-3P

(prepn. and reaction of, in prepn. of leukotriene and lipoxygenase inhibitors)

RN 119161-86-3 USPATFULL

CN 3-Pyridinepropanamine, N-(phenylmethyl)- (9CI) (CA INDEX NAME)



L13 ANSWER 15 OF 17 USPATFULL on STN

Full Text	Chg References
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ACCESSION NUMBER: 91:8812 USPATFULL  
 TITLE: Pyridine-ethanolamine derivatives  
 INVENTOR(S): Alig, Leo, Kaiseraugst, Switzerland  
 Muller, Marcel, Frenkendorf, Switzerland  
 PATENT ASSIGNEE(S): Hoffmann-La Roche Inc., Nutley, NJ, United States (U.S. corporation)

	NUMBER	KIND	DATE
<b>PATENT INFORMATION:</b>	<b>US 4988714</b>		<b>19910129</b>
<b>APPLICATION INFO.:</b>	<b>US 1988-236802</b>		<b>19880826 (7)</b>
<b>RELATED APPLN. INFO.:</b>	Division of Ser. No. <b>US 1987-57150</b> , filed on 3 Jun 1987, now patented, Pat. No. <b>US 4800206</b> , issued on 24 Jan 1989		

	NUMBER	DATE
<b>PRIORITY INFORMATION:</b>	<b>CH 1986-2608</b>	<b>19860627</b>
	<b>CH 1987-1186</b>	<b>19870327</b>
<b>DOCUMENT TYPE:</b>	Utility	
<b>FILE SEGMENT:</b>	Granted	
<b>PRIMARY EXAMINER:</b>	Fan, Jane T.	
<b>LEGAL REPRESENTATIVE:</b>	Gould, George M., Leon, Bernard S., Isgro, William G.	
<b>NUMBER OF CLAIMS:</b>	24	
<b>EXEMPLARY CLAIM:</b>	1	
<b>LINE COUNT:</b>	904	

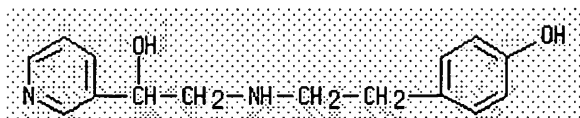
CAS INDEXING IS AVAILABLE FOR THIS PATENT.

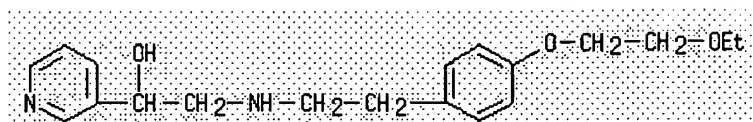
AB Pyridine-ethanolamines of the formula ##STR1## wherein n, X, Y, R<sup>1</sup>, R<sup>2</sup> and R<sup>3</sup> have the significances given in the description, their corresponding enantiomers, diastereomers, and racemates as well as the physiologically compatible salts thereof are described. The compounds of formula I have catabolic activity and can be used for the treatment of obesity and of diabetes mellitus or of conditions which are associated with an increased protein breakdown, or as feed additives for fattening animals. The compounds of formula I can be prepared by alkylating the primary or secondary amines corresponding to the secondary or tertiary amines of formula I.

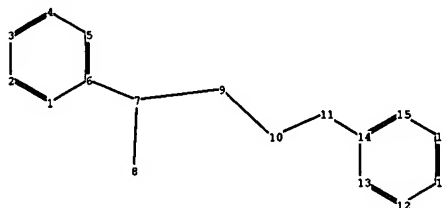
CAS INDEXING IS AVAILABLE FOR THIS PATENT.

IT **115548-43-1P 115626-97-6P**

(prepn. of, as remedy for obesity, diabetes mellitus, and elevated protein degrdn.)

RN **115548-43-1 USPATFULL**CN 3-Pyridinemethanol,  $\alpha$ -[[[2-(4-hydroxyphenyl)ethyl]amino]methyl]- (9CI) (CA INDEX NAME)RN **115626-97-6 USPATFULL**CN 3-Pyridinemethanol,  $\alpha$ -[[[2-[4-(2-ethoxyethoxy)phenyl]ethyl]amino]methyl]- (9CI) (CA INDEX NAME)



























































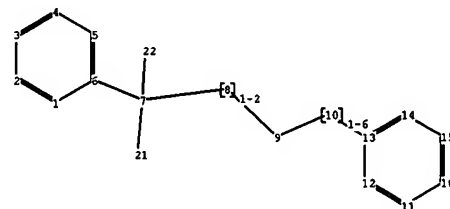




























































































































































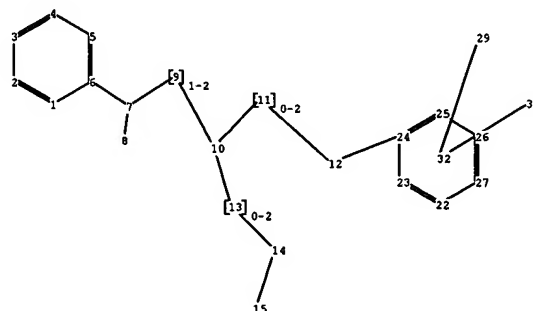

































































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	ENTRY	SESSION
FULL ESTIMATED COST	0.21	0.21

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*
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* effective March 20, 2005. A new display format, IDERL, is now      *
* available and contains the CA role and document type information.  *
*
*****
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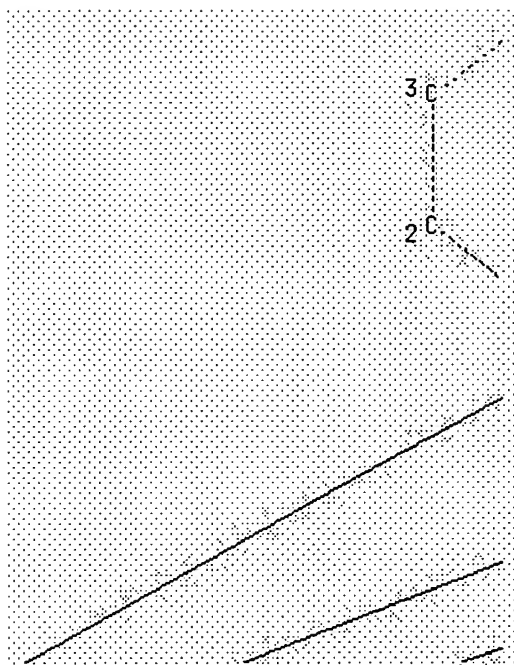
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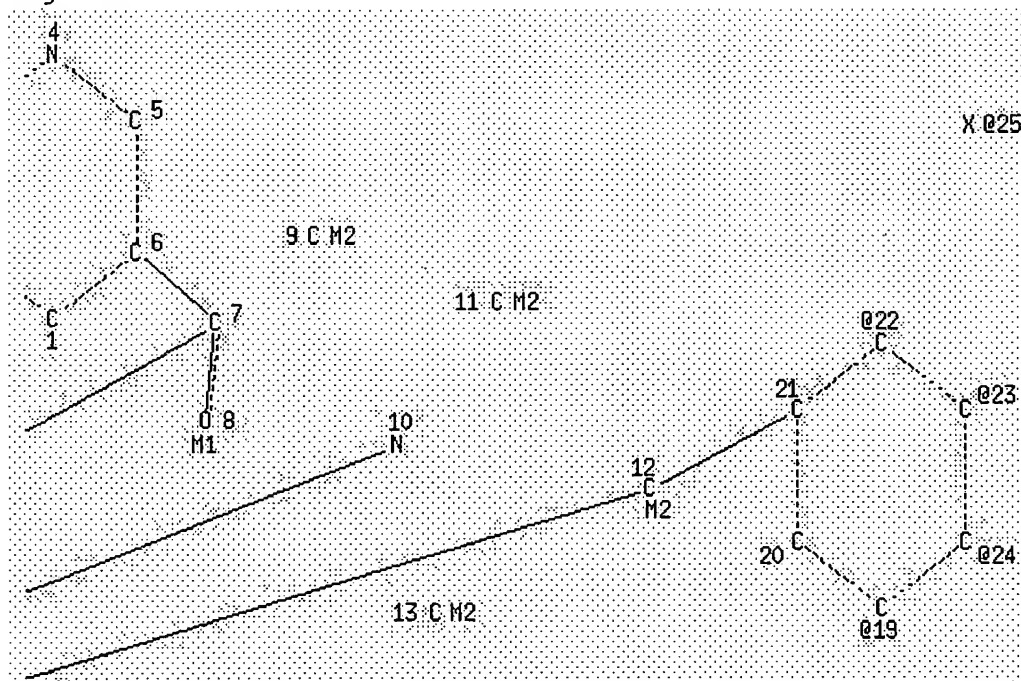
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L1 HAS NO ANSWERS

L1 STR



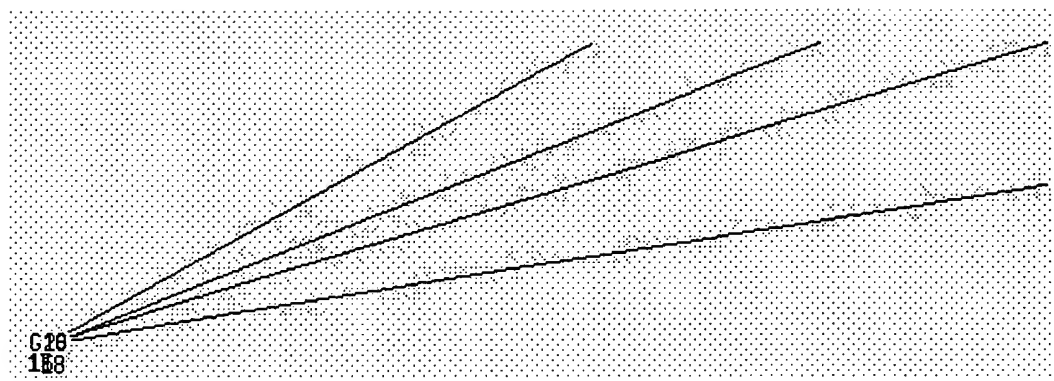
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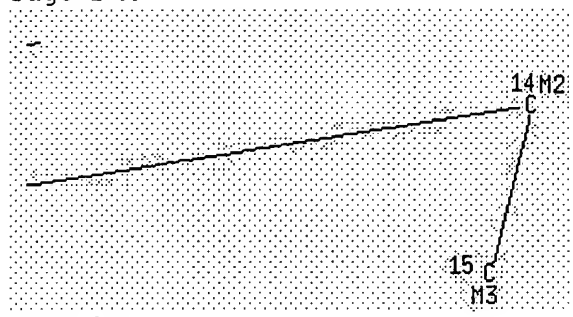
Page 1-B

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Page 1-C



Page 2-A



Page 2-B

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REP G19=(0-2) 11-10 11-12  
REP G20=(0-2) 13-10 13-14

VPA 25-22/23/24 S

VPA 26-19/23/24 S

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 DEFAULT ECLEVEL IS LIMITED

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RSPEC I  
 NUMBER OF NODES IS 26

STEREO ATTRIBUTES: NONE

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SEARCH ENDED BY USER

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 SAMPLE SCREEN SEARCH COMPLETED - 118 TO ITERATE

100.0% PROCESSED 118 ITERATIONS 0 ANSWERS  
 SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*  
 BATCH \*\*COMPLETE\*\*  
 PROJECTED ITERATIONS: 1709 TO 3011  
 PROJECTED ANSWERS: 0 TO 0

L2 0 SEA SSS SAM L1

=> s l1 full

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 FULL SCREEN SEARCH COMPLETED - 2501 TO ITERATE

100.0% PROCESSED 2501 ITERATIONS 3 ANSWERS  
 SEARCH TIME: 00.00.01

L3 3 SEA SSS FUL L1

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COST IN U.S. DOLLARS	SINCE FILE	TOTAL
	ENTRY	SESSION
FULL ESTIMATED COST	170.02	170.23

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FILE LAST UPDATED: 23 May 2006 (20060523/ED)

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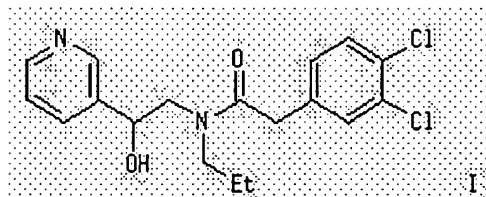
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L4 ANSWER 1 OF 2 HCAPLUS COPYRIGHT 2006 ACS on STN

Full Text

ACCESSION NUMBER: 2005:1306976 HCAPLUS  
DOCUMENT NUMBER: 144:212622  
TITLE: Synthesis, Conformation, and Stereodynamics of a Salt of 2-([2-(3,4-Dichlorophenyl)-ethyl]propylamino)-1-pyridin-3-ylethanol  
AUTHOR(S): Korosec, Tina; Grdadolnik, Joze; Urleb, Uros; Kocjan, Darko; Golic Grdadolnik, Simona  
CORPORATE SOURCE: Drug Discovery, Lek Pharmaceuticals d. d., Ljubljana, SI-1526, Slovenia  
SOURCE: Journal of Organic Chemistry (2006), 71(2), 792-795  
CODEN: JOCEAH; ISSN: 0022-3263  
PUBLISHER: American Chemical Society  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
OTHER SOURCE(S): CASREACT 144:212622  
GI



AB The dihydrobromide salt of [(3,4-dichlorophenylethyl)(propyl)amino]-3-pyridineethanol I is prepd. by two routes; the <sup>1</sup>H NMR spectrum of I·2HBr in methanol-d<sub>4</sub> shows line broadening at room temp. from the equilibration of diastereomers at nitrogen. Redn. of 3-(bromoacetyl)pyridine hydrobromide with sodium borohydride, substitution of the bromide with propylamine, acylation of the secondary amine with 3,4-dichlorophenylacetic acid, amide redn. with borane-dimethyl sulfide, and formation of the dihydrobromide salt yields I·2HBr in five steps and 26% overall yield. Redn. of 3-(bromoacetyl)pyridine hydrobromide with sodium borohydride, substitution of the bromide with 3,4-dichlorophenethylamine, reductive amination with propanal and sodium triacetoxyborohydride in 1,2-dichloroethane, and formation of the dihydrobromide salt yields I·2HBr in four steps and 59% overall yield.

Free energy barriers are detd. for the line broadening processes present in NMR spectra of I?2HBr or in spectra of mixts. of I and benzenesulfonic acid; calcd. structures of the diastereomers of I?H+ are consistent with the results of NOESY and ROESY expts. on I?2HBr.

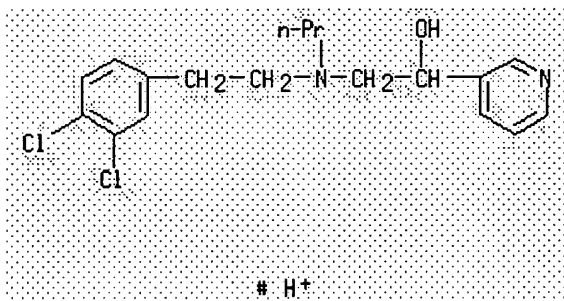
IT **875811-95-3**

RL: PRP (Properties)

(calcd. structure of diastereomers of a protonated tertiary amino-substituted 3-pyridineethanol to det. the source of line broadening in the NMR spectra of the corresponding dihydrobromide salt)

RN **875811-95-3** HCAPLUS

CN 3-Pyridinemethanol,  $\alpha$ -[[[2-(3,4-dichlorophenyl)ethyl]propylamino]methyl]-, conjugate monoacid (9CI) (CA INDEX NAME)



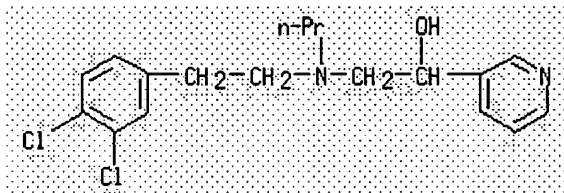
IT **648930-55-6P**

RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(prepn. of the dihydrobromide salt of a tertiary amino-substituted 3-pyridineethanol, its NMR line broadening due to inversion at nitrogen, calcd. free energy barriers to equilibration, and calcd. structures for its diastereomers)

RN **648930-55-6** HCAPLUS

CN 3-Pyridinemethanol,  $\alpha$ -[[[2-(3,4-dichlorophenyl)ethyl]propylamino]methyl]- (9CI) (CA INDEX NAME)



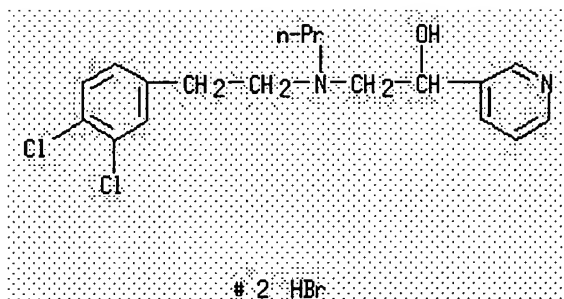
IT **648930-56-7P**

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation) (prepn. of the dihydrobromide salt of a tertiary amino-substituted 3-pyridineethanol, its NMR line broadening due to inversion at nitrogen, calcd. free energy barriers to equilibration, and calcd. structures for its diastereomers)

RN **648930-56-7** HCAPLUS

CN 3-Pyridinemethanol,  $\alpha$ -[[[2-(3,4-dichlorophenyl)ethyl]propylamino]methyl]-, dihydrobromide (9CI) (CA INDEX NAME)





REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

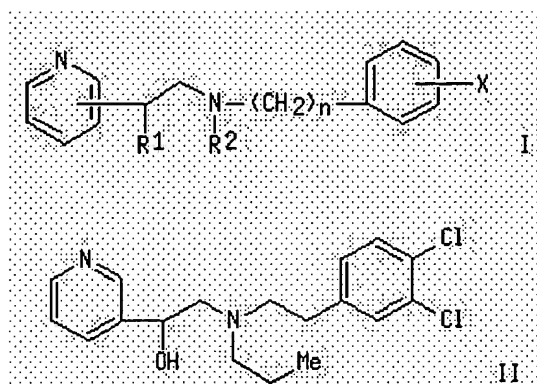
L4 ANSWER 2 OF 2 HCAPLUS COPYRIGHT 2006 ACS on STN

Full  
Text  
References

ACCESSION NUMBER: 2004:60474 HCAPLUS  
DOCUMENT NUMBER: 140:128278  
TITLE: Preparation of 1-pyridyl-2-[(2-phenylethyl)amino]ethanols as inhibitors of cholesterol biosynthesis  
INVENTOR(S): Rode, Breda; Rozman, Damjana; Fon, Tacer Klementina; Kocjan, Darko  
PATENT ASSIGNEE(S): Lek Pharmaceuticals D.D., Slovenia  
SOURCE: PCT Int. Appl., 46 pp.  
CODEN: PIXXD2  
DOCUMENT TYPE: Patent  
LANGUAGE: English  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
<u>WO 2004007456</u>	A1	20040122	<u>WO 2003-SI21</u>	20030709
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
<u>SI 21268</u>	C	20040229	<u>SI 2002-177</u>	20020717
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<u>CA 2493004</u>	AA	20040122	<u>CA 2003-2493004</u>	20030709
<u>AU 2003248614</u>	A1	20040202	<u>AU 2003-248614</u>	20030709
<u>EP 1546105</u>	A1	20050629	<u>EP 2003-764285</u>	20030709
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
<u>BR 2003012945</u>	A	20050712	<u>BR 2003-12945</u>	20030709
<u>CN 1668594</u>	A	20050914	<u>CN 2003-816850</u>	20030709
<u>JP 2005538081</u>	T2	20051215	<u>JP 2004-521370</u>	20030709
<u>NO 2005000833</u>	A	20050418	<u>NO 2005-833</u>	20050216
<u>US 2005256172</u>	A1	20051117	<u>US 2005-521294</u>	20050524
PRIORITY APPLN. INFO.:			<u>SI 2002-177</u>	A 20020717
			<u>SI 2002-287</u>	A 20021128
			<u>WO 2003-SI21</u>	W 20030709
OTHER SOURCE(S):		MARPAT 140:128278		

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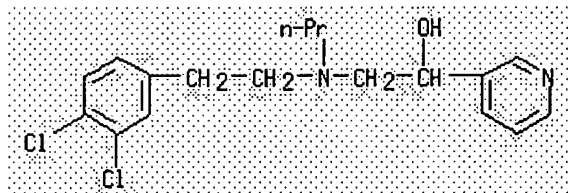
AB Title compds. I [wherein  $n = 1-4$ ;  $R_1 = H, OH, \text{ or alkoxy}$ ;  $R_2 = H \text{ or alkyl}$ ;  $X = H, F, Cl, Br, OH, CF_3, 3,4-Cl_2, 2,4-Cl_2, \text{ or alkoxy}$ ; and the enantiomers, diastereoisomers, racemates, or physiol. acceptable acid addn. salts thereof] were prepd. as ligands of  $\sigma$  receptors for inhibiting cholesterol biosynthesis. For example, reaction of 3-(bromoacetyl)pyridine $\cdot$ HBr with  $NaBH_4$  in abs. EtOH, followed by alkylation with  $PrNH_2$  afforded 1-(3-pyridyl)-2-propylaminoethanol (50%). The amine was coupled with 3,4-dichlorophenylacetic acid in  $CH_2Cl_2$  in the presence of DCC to give 1-(3-pyridyl)-2-[N-[2-(3,4-dichlorophenyl)acetyl]-N-propylamino]ethanol (50%). Redn. of the acetamide using  $LiAlH_4$  in anhyd. THF provided the ethylamine (60%), which was converted to II $\cdot$ 2HBr (BK-35 $\cdot$ 2HBr) in 85% yield. The latter completely blocked cholesterol biosynthesis and showed a ten-fold increase in the accumulation of sterol intermediates of the postsqualene portion of cholesterol biosynthesis. Thus, I and their pharmaceutical compns. are appropriate for the treatment of hypercholesterolemia and hyperlipemia in humans (no data).

IT **648930-55-6P**, 1-(3-Pyridyl)-2-[N-[2-(3,4-dichlorophenyl)ethyl]-N-propylamino]ethanol **648930-56-7P**, 1-(3-Pyridyl)-2-[N-[2-(3,4-dichlorophenyl)ethyl]-N-propylamino]ethanol dihydrobromide  
 RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(anticholesteremic agent; prepn. of pyridyl(phenylethylamino)ethanols as inhibitors of cholesterol biosynthesis for treatment of hypercholesterolemia and hyperlipemia)

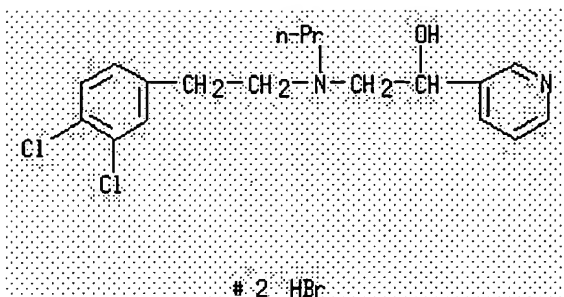
RN **648930-55-6** HCAPLUS

CN 3-Pyridinemethanol,  $\alpha$ -[[[2-(3,4-dichlorophenyl)ethyl]propylamino]methyl]- (9CI) (CA INDEX NAME)



RN **648930-56-7** HCAPLUS

CN 3-Pyridinemethanol,  $\alpha$ -[[[2-(3,4-dichlorophenyl)ethyl]propylamino]methyl]-, dihydrobromide (9CI) (CA INDEX NAME)



REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> file caold

COST IN U.S. DOLLARS

SINCE FILE	TOTAL
ENTRY	SESSION

FULL ESTIMATED COST

12.75	182.98
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DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE	TOTAL
ENTRY	SESSION

CA SUBSCRIBER PRICE

-1.50	-1.50
-------	-------

FILE 'CAOLD' ENTERED AT 11:49:03 ON 24 MAY 2006

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FILE COVERS 1907-1966

FILE LAST UPDATED: 01 May 1997 (19970501/UP)

This file contains CAS Registry Numbers for easy and accurate substance identification. Title keywords, authors, patent assignees, and patent information, e.g., patent numbers, are now searchable from 1907-1966. TIFF images of CA abstracts printed between 1907-1966 are available in the PAGE display formats.

New CAS Information Use Policies, enter HELP USAGETERMS for details.

This file supports REGISTRY for direct browsing and searching of all substance data from the REGISTRY file. Enter HELP FIRST for more information.

=> d his

(FILE 'HOME' ENTERED AT 11:43:32 ON 24 MAY 2006)

FILE 'REGISTRY' ENTERED AT 11:43:51 ON 24 MAY 2006

L1 STRUCTURE UPLOADED

L2 0 S L1

L3 3 S L1 FULL

FILE 'HCAPLUS' ENTERED AT 11:48:31 ON 24 MAY 2006

L4 2 S L3

FILE 'CAOLD' ENTERED AT 11:49:03 ON 24 MAY 2006

=> s 13

L5 0 L3

```
=> file hcaplus
COST IN U.S. DOLLARS          SINCE FILE      TOTAL
                                ENTRY      SESSION
FULL ESTIMATED COST          0.44      183.42

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)  SINCE FILE      TOTAL
                                                ENTRY      SESSION
CA SUBSCRIBER PRICE          0.00      -1.50
```

FILE 'HCAPLUS' ENTERED AT 11:49:36 ON 24 MAY 2006  
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FILE COVERS 1907 - 24 May 2006 VOL 144 ISS 22  
 FILE LAST UPDATED: 23 May 2006 (20060523/ED)

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This file contains CAS Registry Numbers for easy and accurate substance identification.

```
=> s rode, b?/au and rozman, d?/au and tacer, k?/au and kocjan, d?/au
    377 RODE, B?/AU
    56 ROZMAN, D?/AU
    3 TACER, K?/AU
    69 KOCJAN, D?/AU
L6      0 RODE, B?/AU AND ROZMAN, D?/AU AND TACER, K?/AU AND KOCJAN, D?/AU
```

```
=>
Uploading structure
```

```
L7      STRUCTURE UPLOADED
```

```
=> s 17
REGISTRY INITIATED
Substance data SEARCH and crossover from CAS REGISTRY in progress...
Use DISPLAY HITSTR (or FHITSTR) to directly view retrieved structures.
```

```
SAMPLE SEARCH INITIATED 11:55:24 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 964 TO ITERATE
```

```
100.0% PROCESSED          964 ITERATIONS          0 ANSWERS
SEARCH TIME: 00.00.01
```

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*  
 BATCH \*\*COMPLETE\*\*  
 PROJECTED ITERATIONS: 17418 TO 21142  
 PROJECTED ANSWERS: 0 TO 0

L8 0 SEA SSS SAM L7

L9 0 L8

=> file reg

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	2.53	211.69
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	0.00	-1.50

FILE 'REGISTRY' ENTERED AT 11:55:28 ON 24 MAY 2006  
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STRUCTURE FILE UPDATES: 23 MAY 2006 HIGHEST RN 885357-09-5  
 DICTIONARY FILE UPDATES: 23 MAY 2006 HIGHEST RN 885357-09-5

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TSCA INFORMATION NOW CURRENT THROUGH January 6, 2006

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\*\*\*\*\*  
 \*  
 \* The CA roles and document type information have been removed from \*  
 \* the IDE default display format and the ED field has been added, \*  
 \* effective March 20, 2005. A new display format, IDERL, is now \*  
 \* available and contains the CA role and document type information. \*  
 \*  
 \*\*\*\*\*

Structure search iteration limits have been increased. See HELP SLIMITS for details.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

<http://www.cas.org/ONLINE/UG/regprops.html>

=>

Uploading structure

L10        STRUCTURE UPLOADED

=> s l10

SAMPLE SEARCH INITIATED 11:55:40 FILE 'REGISTRY'  
SAMPLE SCREEN SEARCH COMPLETED -        964 TO ITERATE

100.0% PROCESSED        964 ITERATIONS        0 ANSWERS  
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:   ONLINE   \*\*COMPLETE\*\*  
                             BATCH   \*\*COMPLETE\*\*  
PROJECTED ITERATIONS:        17418 TO        21142  
PROJECTED ANSWERS:            0 TO        0

L11        0 SEA SSS SAM L10

=> s l10 full

THE ESTIMATED SEARCH COST FOR FILE 'REGISTRY' IS 166.50 U.S. DOLLARS  
DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END:y  
FULL SEARCH INITIATED 11:55:45 FILE 'REGISTRY'  
FULL SCREEN SEARCH COMPLETED -        18828 TO ITERATE

100.0% PROCESSED        18828 ITERATIONS        1 ANSWERS  
SEARCH TIME: 00.00.01

L12        1 SEA SSS FUL L10

=> file hcaplus

COST IN U.S. DOLLARS	SINCE FILE	TOTAL
	ENTRY	SESSION
FULL ESTIMATED COST	166.94	378.63
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE	TOTAL
	ENTRY	SESSION
CA SUBSCRIBER PRICE	0.00	-1.50

FILE 'HCAPLUS' ENTERED AT 11:55:48 ON 24 MAY 2006  
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.  
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FILE COVERS 1907 - 24 May 2006 VOL 144 ISS 22  
FILE LAST UPDATED: 23 May 2006 (20060523/ED)

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This file contains CAS Registry Numbers for easy and accurate substance identification.

=&gt; s 112

L13 1 L12

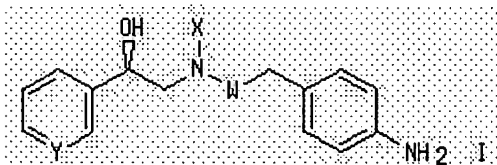
=&gt; d 113, ibib abs hitstr, 1

L13 ANSWER 1 OF 1 HCAPLUS COPYRIGHT 2006 ACS on STN

Full Text	CHIRP References
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ACCESSION NUMBER: 1998:632236 HCAPLUS  
 DOCUMENT NUMBER: 129:202860  
 TITLE: Preparation of N-Boc-N-(R)-2-((3-pyridyl)-2-hydroxyethyl-N-2-(4-aminophenyl)ethylamine and 2-(4-aminophenyl)-N-2-R-hydroxy-2-pyridine-3-yl-ethyl)acetamide  
 INVENTOR(S): Zhao, Dalian; Chartrain, Michel M.; Chung, John Y. L.; Roberge, Christopher  
 PATENT ASSIGNEE(S): Merck and Co., Inc., USA  
 SOURCE: Brit. UK Pat. Appl., 29 pp.  
 CODEN: BAXXDU  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
<u>GB 2315748</u>	A1	19980211	<u>GB 1997-14800</u>	19970714
<u>PRIORITY APPLN. INFO.:</u>			<u>US 1996-22056P</u>	P 19960722
<u>OTHER SOURCE(S):</u>	CASREACT 129:202860; MARPAT 129:202860			
GI				



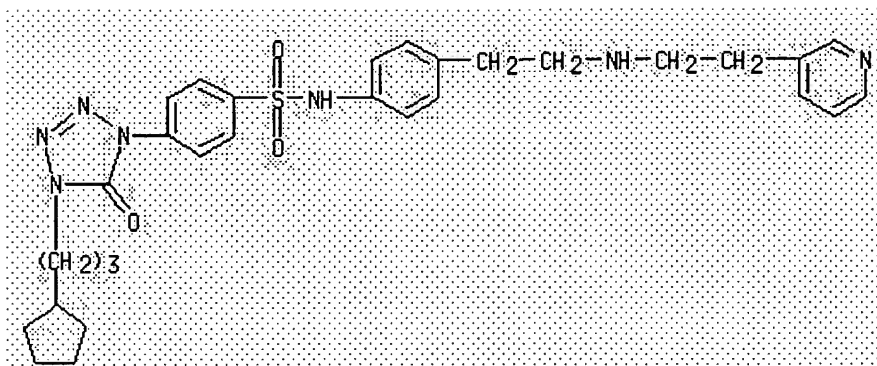
AB The title compds. (I; X = H, Boc; W = CH<sub>2</sub>, CO; Y = CH, N) are prepd. by multi-step reactions from 3-acetylpyridine in an overall good yield. I are useful as intermediates in the prodn. of  $\beta$ -3 agonist for the treatment of obesity and diabetes (no data).

IT **212253-89-9P**

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PNU (Preparation, unclassified); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
 (prepn. of N-Boc-N-(R)-2-((3-pyridyl)-2-hydroxyethyl-N-2-(4-aminophenyl)ethylamine and 2-(4-aminophenyl)-N-2-R-hydroxy-2-pyridine-3-yl-ethyl)acetamide)

RN **212253-89-9** HCAPLUS

CN Benzenesulfonamide, 4-[4-(3-cyclopentylpropyl)-4,5-dihydro-5-oxo-1H-tetrazol-1-yl]-N-[4-[2-[[2-(3-pyridinyl)ethyl]amino]ethyl]phenyl]- (9CI)  
 (CA INDEX NAME)



=> file caold  
COST IN U.S. DOLLARS

SINCE FILE	TOTAL
ENTRY	SESSION
10.17	388.80

FULL ESTIMATED COST

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE	TOTAL
ENTRY	SESSION
-0.75	-2.25

CA SUBSCRIBER PRICE

FILE 'CAOLD' ENTERED AT 11:57:03 ON 24 MAY 2006  
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FILE COVERS 1907-1966

FILE LAST UPDATED: 01 May 1997 (19970501/UP)

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=> d his

(FILE 'HOME' ENTERED AT 11:43:32 ON 24 MAY 2006)

FILE 'REGISTRY' ENTERED AT 11:43:51 ON 24 MAY 2006

L1	STRUCTURE UPLOADED
L2	0 S L1
L3	3 S L1 FULL

FILE 'HCAPLUS' ENTERED AT 11:48:31 ON 24 MAY 2006

L4	2 S L3
----	--------

FILE 'CAOLD' ENTERED AT 11:49:03 ON 24 MAY 2006

L5	0 S L3
----	--------

FILE 'HCAPLUS' ENTERED AT 11:49:36 ON 24 MAY 2006



L6 0 S RODE, B?/AU AND ROZMAN, D?/AU AND TACER, K?/AU AND KOCJAN, D?  
 L7 STRUCTURE UPLOADED  
 S L7

FILE 'REGISTRY' ENTERED AT 11:55:24 ON 24 MAY 2006  
 L8 0 S L7

FILE 'HCAPLUS' ENTERED AT 11:55:24 ON 24 MAY 2006  
 L9 0 S L8

FILE 'REGISTRY' ENTERED AT 11:55:28 ON 24 MAY 2006  
 L10 STRUCTURE UPLOADED  
 L11 0 S L10  
 L12 1 S L10 FULL

FILE 'HCAPLUS' ENTERED AT 11:55:48 ON 24 MAY 2006  
 L13 1 S L12

FILE 'CAOLD' ENTERED AT 11:57:03 ON 24 MAY 2006

=> s l12

L14 0 L12

=> file reg

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.44	389.24
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	0.00	-2.25

FILE 'REGISTRY' ENTERED AT 11:57:10 ON 24 MAY 2006  
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STRUCTURE FILE UPDATES: 23 MAY 2006 HIGHEST RN 885357-09-5  
 DICTIONARY FILE UPDATES: 23 MAY 2006 HIGHEST RN 885357-09-5

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TSCA INFORMATION NOW CURRENT THROUGH January 6, 2006

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\*\*\*\*\*  
 \*  
 \* The CA roles and document type information have been removed from \*  
 \* the IDE default display format and the ED field has been added, \*  
 \* effective March 20, 2005. A new display format, IDERL, is now \*  
 \* available and contains the CA role and document type information. \*  
 \*  
 \*\*\*\*\*

Structure search iteration limits have been increased. See HELP SLIMITS

for details.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

<http://www.cas.org/ONLINE/UG/regprops.html>

=>

Uploading structure

L15        STRUCTURE UPLOADED

=> s l15

SAMPLE SEARCH INITIATED 12:01:49 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED -        1544 TO ITERATE

100.0% PROCESSED        1544 ITERATIONS

50 ANSWERS

INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:    ONLINE    \*\*COMPLETE\*\*

BATCH    \*\*COMPLETE\*\*

PROJECTED ITERATIONS:        28523 TO        33237

PROJECTED ANSWERS:            800 TO        1760

L16        50 SEA SSS SAM L15

=> s l15 full

THE ESTIMATED SEARCH COST FOR FILE 'REGISTRY' IS 166.50 U.S. DOLLARS

DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END:y

FULL SEARCH INITIATED 12:01:59 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED -        30140 TO ITERATE

100.0% PROCESSED        30140 ITERATIONS

1202 ANSWERS

SEARCH TIME: 00.00.01

L17        1202 SEA SSS FUL L15

=> file hcaplus

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

170.02

559.26

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE

TOTAL

ENTRY

SESSION

CA SUBSCRIBER PRICE

0.00

-2.25

FILE 'HCAPLUS' ENTERED AT 12:02:03 ON 24 MAY 2006

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FILE LAST UPDATED: 23 May 2006 (20060523/ED)

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This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s l17

L18 107 L17

=> s l18 and rode, b?/au

377 RODE, B?/AU

L19 1 L18 AND RODE, B?/AU

=> d his

(FILE 'HOME' ENTERED AT 11:43:32 ON 24 MAY 2006)

FILE 'REGISTRY' ENTERED AT 11:43:51 ON 24 MAY 2006

L1 STRUCTURE UPLOADED

L2 0 S L1

L3 3 S L1 FULL

FILE 'HCAPLUS' ENTERED AT 11:48:31 ON 24 MAY 2006

L4 2 S L3

FILE 'CAOLD' ENTERED AT 11:49:03 ON 24 MAY 2006

L5 0 S L3

FILE 'HCAPLUS' ENTERED AT 11:49:36 ON 24 MAY 2006

L6 0 S RODE, B?/AU AND ROZMAN, D?/AU AND TACER, K?/AU AND KOCJAN, D?

L7 STRUCTURE UPLOADED

S L7

FILE 'REGISTRY' ENTERED AT 11:55:24 ON 24 MAY 2006

L8 0 S L7

FILE 'HCAPLUS' ENTERED AT 11:55:24 ON 24 MAY 2006

L9 0 S L8

FILE 'REGISTRY' ENTERED AT 11:55:28 ON 24 MAY 2006

L10 STRUCTURE UPLOADED

L11 0 S L10

L12 1 S L10 FULL

FILE 'HCAPLUS' ENTERED AT 11:55:48 ON 24 MAY 2006

L13 1 S L12

FILE 'CAOLD' ENTERED AT 11:57:03 ON 24 MAY 2006

L14 0 S L12

FILE 'REGISTRY' ENTERED AT 11:57:10 ON 24 MAY 2006

L15 STRUCTURE UPLOADED

L16 50 S L15

L17 1202 S L15 FULL

FILE 'HCAPLUS' ENTERED AT 12:02:03 ON 24 MAY 2006

L18 107 S L17

L19 1 S L18 AND RODE, B?/AU

=> s 112 not 119

1 L12

L20 1 L12 NOT L19

=> s 120 not 113

L21 0 L20 NOT L13

=> s 118 and rozman, d?/au

56 ROZMAN, D?/AU

L22 1 L18 AND ROZMAN, D?/AU

=> d 122, ibib abs hitstr, 1

L22 ANSWER 1 OF 1 HCAPLUS COPYRIGHT 2006 ACS on STN

Full  
Text

Citing  
References

ACCESSION NUMBER: 2004:60474 HCAPLUS

DOCUMENT NUMBER: 140:128278

TITLE: Preparation of 1-pyridyl-2-[(2-phenylethyl)amino]ethanols as inhibitors of cholesterol biosynthesis

INVENTOR(S): Rode, Breda; **Rozman, Damjana**; Fon, Tacer Klementina; Kocjan, Darko

PATENT ASSIGNEE(S): Lek Pharmaceuticals D.D., Slovenia

SOURCE: PCT Int. Appl., 46 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
<u>WO 2004007456</u>	A1	20040122	<u>WO 2003-SI21</u>	20030709
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
<u>SI 21268</u>	C	20040229	<u>SI 2002-177</u>	20020717
<u>SI 21368</u>	C	20040630	<u>SI 2002-287</u>	20021128
<u>CA 2493004</u>	AA	20040122	<u>CA 2003-2493004</u>	20030709
<u>AU 2003248614</u>	A1	20040202	<u>AU 2003-248614</u>	20030709
<u>EP 1546105</u>	A1	20050629	<u>EP 2003-764285</u>	20030709
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
<u>BR 2003012945</u>	A	20050712	<u>BR 2003-12945</u>	20030709
<u>CN 1668594</u>	A	20050914	<u>CN 2003-816850</u>	20030709
<u>JP 2005538081</u>	T2	20051215	<u>JP 2004-521370</u>	20030709

NO 2005000833

A 20050418

NO 2005-833

20050216

US 2005256172

A1 20051117

US 2005-521294

20050524

PRIORITY APPLN. INFO.:

SI 2002-177

A 20020717

SI 2002-287

A 20021128

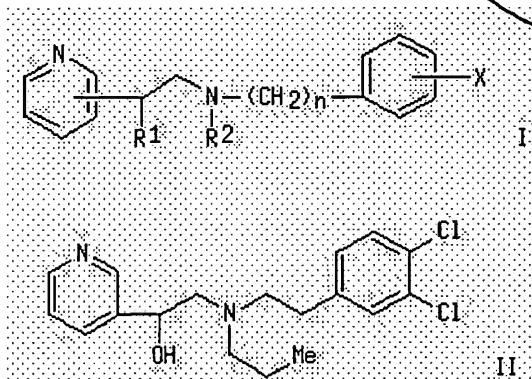
WO 2003-SI21

W 20030709

OTHER SOURCE(S):

MARPAT 140:128278

GI



10521294

AB Title compds. I [wherein  $n = 1-4$ ;  $R_1 = H, OH$ , or alkoxy;  $R_2 = H$  or alkyl;  $X = H, F, Cl, Br, OH, CF_3, 3,4-Cl_2, 2,4-Cl_2$ , or alkoxy; and the enantiomers, diastereoisomers, racemates, or physiol. acceptable acid addn. salts thereof] were prep'd. as ligands of  $\sigma$  receptors for inhibiting cholesterol biosynthesis. For example, reaction of 3-(bromoacetyl)pyridine·HBr with  $NaBH_4$  in abs. EtOH, followed by alkylation with  $PrNH_2$  afforded 1-(3-pyridyl)-2-propylaminoethanol (50%). The amine was coupled with 3,4-dichlorophenylacetic acid in  $CH_2Cl_2$  in the presence of DCC to give 1-(3-pyridyl)-2-[N-[2-(3,4-dichlorophenyl)acetyl]-N-propylamino]ethanol (50%). Redn. of the acetamide using  $LiAlH_4$  in anhyd. THF provided the ethylamine (60%), which was converted to II·2HBr (BK-35·2HBr) in 85% yield. The latter completely blocked cholesterol biosynthesis and showed a ten-fold increase in the accumulation of sterol intermediates of the postsqualene portion of cholesterol biosynthesis. Thus, I and their pharmaceutical compns. are appropriate for the treatment of hypercholesterolemia and hyperlipemia in humans (no data).

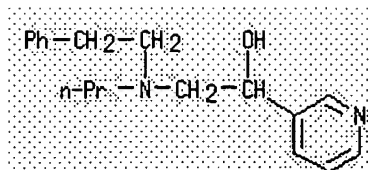
IT 648930-50-1P, 1-(3-Pyridyl)-2-[N-(2-phenylethyl)-N-propylamino]ethanol 648930-51-2P, 1-(3-Pyridyl)-2-[N-(2-phenylethyl)-N-propylamino]ethanol dihydrobromide 648930-53-4P, 1-(3-Pyridyl)-2-[N-[2-(3,4-dichlorophenyl)ethyl]-N-methylamino]ethanol 648930-54-5P, 1-(3-Pyridyl)-2-[N-[2-(3,4-dichlorophenyl)ethyl]-N-methylamino]ethanol dihydrobromide 648930-55-6P, 1-(3-Pyridyl)-2-[N-[2-(3,4-dichlorophenyl)ethyl]-N-propylamino]ethanol 648930-56-7P, 1-(3-Pyridyl)-2-[N-[2-(3,4-dichlorophenyl)ethyl]-N-propylamino]ethanol dihydrobromide

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(anticholesteremic agent; prepn. of pyridyl(phenylethylamino)ethanols as inhibitors of cholesterol biosynthesis for treatment of hypercholesterolemia and hyperlipemia)

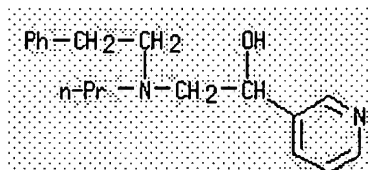
RN 648930-50-1 HCAPLUS

CN 3-Pyridinemethanol,  $\alpha$ -[[2-(phenylethyl)propylamino]methyl]- (9CI)  
(CA INDEX NAME)



RN 648930-51-2 HCAPLUS

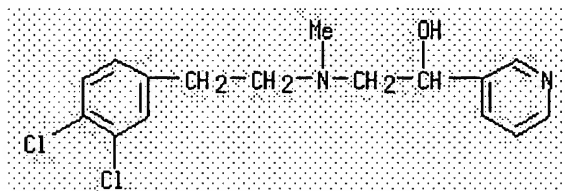
CN 3-Pyridinemethanol,  $\alpha$ -[[2-(2-phenylethyl)propylamino]methyl]-, dihydrobromide (9CI) (CA INDEX NAME)



# 2 HBr

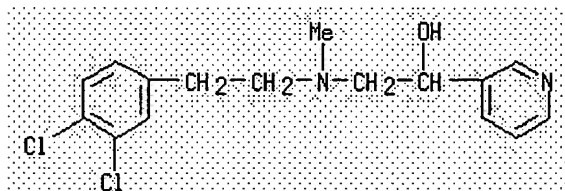
RN 648930-53-4 HCAPLUS

CN 3-Pyridinemethanol,  $\alpha$ -[[[2-(3,4-dichlorophenyl)ethyl]methylamino]methyl]- (9CI) (CA INDEX NAME)



RN 648930-54-5 HCAPLUS

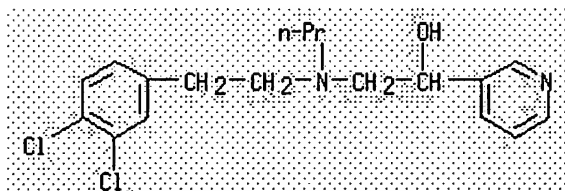
CN 3-Pyridinemethanol,  $\alpha$ -[[[2-(3,4-dichlorophenyl)ethyl]methylamino]methyl]-, dihydrobromide (9CI) (CA INDEX NAME)



# 2 HBr

RN 648930-55-6 HCAPLUS

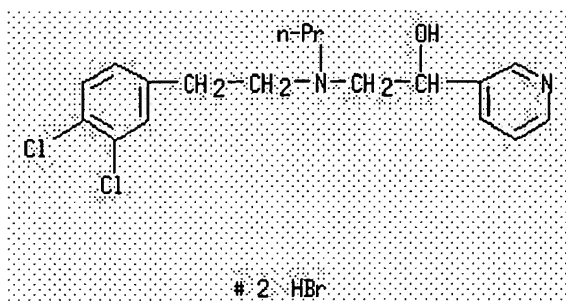
CN 3-Pyridinemethanol,  $\alpha$ -[[[2-(3,4-dichlorophenyl)ethyl]propylamino]methyl]- (9CI) (CA INDEX NAME)



RN 648930-56-7 HCAPLUS

CN 3-Pyridinemethanol,  $\alpha$ -[[[2-(3,4-dichlorophenyl)ethyl]propylamino]methyl]- (9CI) (CA INDEX NAME)

hyl]-, dihydrobromide (9CI) (CA INDEX NAME)



REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

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(FILE 'HOME' ENTERED AT 11:43:32 ON 24 MAY 2006)

FILE 'REGISTRY' ENTERED AT 11:43:51 ON 24 MAY 2006

L1 STRUCTURE UPLOADED  
L2 0 S L1  
L3 3 S L1 FULL

FILE 'HCAPLUS' ENTERED AT 11:48:31 ON 24 MAY 2006

L4 2 S L3

FILE 'CAOLD' ENTERED AT 11:49:03 ON 24 MAY 2006

L5 0 S L3

FILE 'HCAPLUS' ENTERED AT 11:49:36 ON 24 MAY 2006

L6 0 S RODE, B?/AU AND ROZMAN, D?/AU AND TACER, K?/AU AND KOCJAN, D?  
L7 STRUCTURE UPLOADED  
S L7

FILE 'REGISTRY' ENTERED AT 11:55:24 ON 24 MAY 2006

L8 0 S L7

FILE 'HCAPLUS' ENTERED AT 11:55:24 ON 24 MAY 2006

L9 0 S L8

FILE 'REGISTRY' ENTERED AT 11:55:28 ON 24 MAY 2006

L10 STRUCTURE UPLOADED  
L11 0 S L10  
L12 1 S L10 FULL

FILE 'HCAPLUS' ENTERED AT 11:55:48 ON 24 MAY 2006

L13 1 S L12

FILE 'CAOLD' ENTERED AT 11:57:03 ON 24 MAY 2006

L14 0 S L12

FILE 'REGISTRY' ENTERED AT 11:57:10 ON 24 MAY 2006

L15 STRUCTURE UPLOADED  
L16 50 S L15  
L17 1202 S L15 FULL

FILE 'HCAPLUS' ENTERED AT 12:02:03 ON 24 MAY 2006

L18 107 S L17  
 L19 1 S L18 AND RODE, B?/AU  
 L20 1 S L12 NOT L19  
 L21 0 S L20 NOT L13  
 L22 1 S L18 AND ROZMAN, D?/AU

=> s l18 not l22  
 L23 106 L18 NOT L22

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 2 FON TACER, K?/AU  
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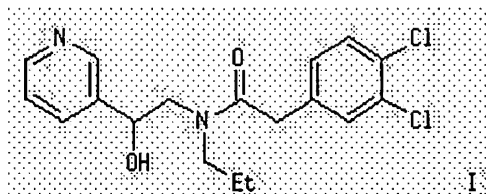
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 69 KOCJAN, D?/AU  
 L25 1 L23 AND KOCJAN, D?/AU

=> d l25, ibib abs hitstr, 1

L25 ANSWER 1 OF 1 HCAPLUS COPYRIGHT 2006 ACS on STN

Full Text  
 Citing References

ACCESSION NUMBER: 2005:1306976 HCAPLUS  
 DOCUMENT NUMBER: 144:212622  
 TITLE: Synthesis, Conformation, and Stereodynamics of a Salt of 2-([2-(3,4-Dichlorophenyl)-ethyl]propylamino)-1-pyridin-3-ylethanol  
 AUTHOR(S): Korosec, Tina; Grdadolnik, Joze; Urleb, Uros; **Kocjan, Darko**; Golic Grdadolnik, Simona  
 CORPORATE SOURCE: Drug Discovery, Lek Pharmaceuticals d. d., Ljubljana, SI-1526, Slovenia  
 SOURCE: Journal of Organic Chemistry (2006), 71(2), 792-795  
 CODEN: JOCEAH; ISSN: 0022-3263  
 PUBLISHER: American Chemical Society  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 OTHER SOURCE(S): CASREACT 144:212622  
 GI



AB The dihydrobromide salt of [(3,4-dichlorophenylethyl)(propyl)amino]-3-pyridineethanol I is prep'd. by two routes; the <sup>1</sup>H NMR spectrum of I·2HBr in methanol-d<sub>4</sub> shows line broadening at room temp. from the equilibration of diastereomers at nitrogen. Redn. of 3-(bromoacetyl)pyridine hydrobromide with sodium borohydride, substitution of the bromide with propylamine, acylation of the secondary amine with 3,4-dichlorophenylacetic acid, amide redn. with borane-dimethyl sulfide, and formation of the dihydrobromide salt yields I·2HBr in five steps and 26% overall yield. Redn. of 3-(bromoacetyl)pyridine hydrobromide with sodium borohydride, substitution of the bromide with 3,4-dichlorophenethylamine, reductive amination with propanal and sodium triacetoxyborohydride in 1,2-dichloroethane, and formation of the



dihydrobromide salt yields I?2HBr in four steps and 59% overall yield. Free energy barriers are detd. for the line broadening processes present in NMR spectra of I?2HBr or in spectra of mixts. of I and benzenesulfonic acid; calcd. structures of the diastereomers of I?H<sup>+</sup> are consistent with the results of NOESY and ROESY expts. on I?2HBr.

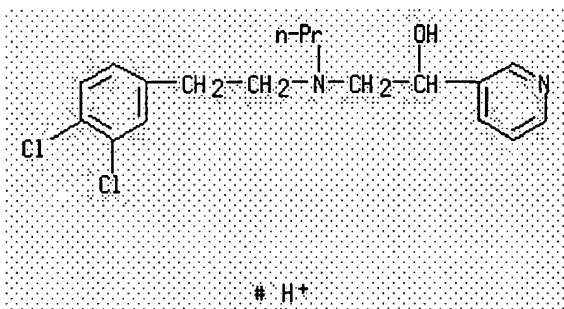
IT **875811-95-3**

RL: PRP (Properties)

(calcd. structure of diastereomers of a protonated tertiary amino-substituted 3-pyridineethanol to det. the source of line broadening in the NMR spectra of the corresponding dihydrobromide salt)

RN **875811-95-3** HCAPLUS

CN 3-Pyridinemethanol,  $\alpha$ -[[[2-(3,4-dichlorophenyl)ethyl]propylamino]methyl]-, conjugate monoacid (9CI) (CA INDEX NAME)

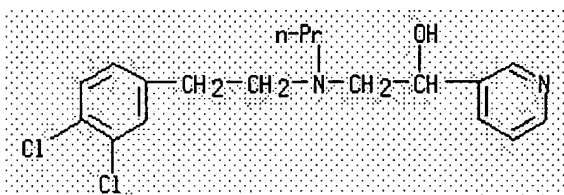
IT **648930-55-6P**

RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(prepn. of the dihydrobromide salt of a tertiary amino-substituted 3-pyridineethanol, its NMR line broadening due to inversion at nitrogen, calcd. free energy barriers to equilibration, and calcd. structures for its diastereomers)

RN **648930-55-6** HCAPLUS

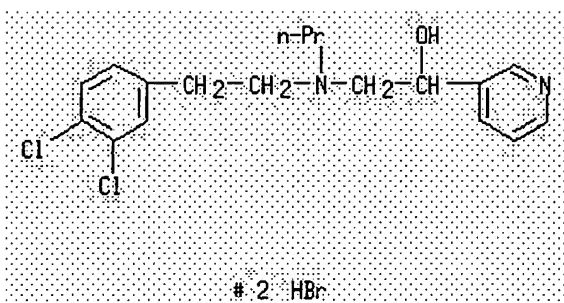
CN 3-Pyridinemethanol,  $\alpha$ -[[[2-(3,4-dichlorophenyl)ethyl]propylamino]methyl]- (9CI) (CA INDEX NAME)

IT **648930-56-7P**

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation) (prepn. of the dihydrobromide salt of a tertiary amino-substituted 3-pyridineethanol, its NMR line broadening due to inversion at nitrogen, calcd. free energy barriers to equilibration, and calcd. structures for its diastereomers)

RN **648930-56-7** HCAPLUS

CN 3-Pyridinemethanol,  $\alpha$ -[[[2-(3,4-dichlorophenyl)ethyl]propylamino]methyl]-, dihydrobromide (9CI) (CA INDEX NAME)



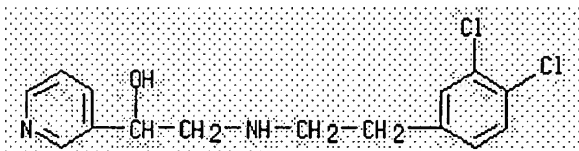
IT 875811-94-2P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(prepn. of the dihydrobromide salt of a tertiary amino-substituted 3-pyridineethanol, its NMR line broadening due to inversion at nitrogen, calcd. free energy barriers to equilibration, and calcd. structures for its diastereomers)

RN 875811-94-2 HCAPLUS

CN 3-Pyridinemethanol,  $\alpha$ -[[[2-(3,4-dichlorophenyl)ethyl]amino]methyl]-(9CI) (CA INDEX NAME)



REFERENCE COUNT:

6

THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=&gt; file caold

COST IN U.S. DOLLARS

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FILE COVERS 1907-1966

FILE LAST UPDATED: 01 May 1997 (19970501/UP)

This file contains CAS Registry Numbers for easy and accurate substance identification. Title keywords, authors, patent assignees, and patent information, e.g., patent numbers, are now searchable from 1907-1966. TIFF images of CA abstracts printed between 1907-1966 are available in the PAGE display formats.

New CAS Information Use Policies, enter HELP USAGETERMS for details.

This file supports REGISTRY for direct browsing and searching of all substance data from the REGISTRY file. Enter HELP FIRST for more information.

=> d his

(FILE 'HOME' ENTERED AT 11:43:32 ON 24 MAY 2006)

FILE 'REGISTRY' ENTERED AT 11:43:51 ON 24 MAY 2006

L1 STRUCTURE UPLOADED

L2 0 S L1

L3 3 S L1 FULL

FILE 'HCAPLUS' ENTERED AT 11:48:31 ON 24 MAY 2006

L4 2 S L3

FILE 'CAOLD' ENTERED AT 11:49:03 ON 24 MAY 2006

L5 0 S L3

FILE 'HCAPLUS' ENTERED AT 11:49:36 ON 24 MAY 2006

L6 0 S RODE, B?/AU AND ROZMAN, D?/AU AND TACER, K?/AU AND KOCJAN, D?

L7 STRUCTURE UPLOADED

S L7

FILE 'REGISTRY' ENTERED AT 11:55:24 ON 24 MAY 2006

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FILE 'REGISTRY' ENTERED AT 11:55:28 ON 24 MAY 2006

L10 STRUCTURE UPLOADED

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L12 1 S L10 FULL

FILE 'HCAPLUS' ENTERED AT 11:55:48 ON 24 MAY 2006

L13 1 S L12

FILE 'CAOLD' ENTERED AT 11:57:03 ON 24 MAY 2006

L14 0 S L12

FILE 'REGISTRY' ENTERED AT 11:57:10 ON 24 MAY 2006

L15 STRUCTURE UPLOADED

L16 50 S L15

L17 1202 S L15 FULL

FILE 'HCAPLUS' ENTERED AT 12:02:03 ON 24 MAY 2006

L18 107 S L17

L19 1 S L18 AND RODE, B?/AU

L20 1 S L12 NOT L19

L21 0 S L20 NOT L13

L22 1 S L18 AND ROZMAN, D?/AU

L23 106 S L18 NOT L22

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FILE 'CAOLD' ENTERED AT 12:05:21 ON 24 MAY 2006

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L26 2 L17

=> d l26, all, 1-2

L26 ANSWER 1 OF 2 CAOLD COPYRIGHT 2006 ACS on STN

Full  
Text

AN CA58:13927d CAOLD  
 TI analgesic isoquinolines  
 AU Kuehne, Martin E.  
 DT Patent  
 TI isoquinolines (analgesic)  
 PA CIBA Ltd.  
 DT Patent

PATENT NO.	KIND	DATE
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PI	BE 617937					
	FR 1336696					
	US 3133926		1964			
IT	<u>1039-95-8</u>	<u>1039-96-9</u>	<u>1043-69-2</u>	<u>1096-86-2</u>	<u>1429-61-4</u>	<u>3949-44-8</u>
	<u>3951-64-2</u>	<u>4461-02-3</u>	<u>25932-48-3</u>	<u>93013-37-7</u>	<u>93947-69-4</u>	<u>93947-70-7</u>

L26 ANSWER 2 OF 2 CAOLD COPYRIGHT 2006 ACS on STN

AN **CA56:2415e** CAOLD  
 TI synthesis of pyridine derivs. with potential circulatory action  
 AU Zymalkowski, Felix; Koppe, F.

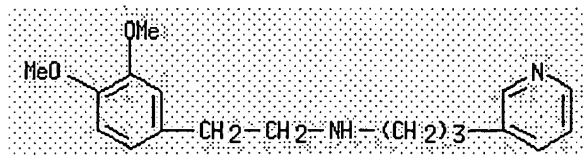
IT	<u>3737-69-7</u>	<u>19730-15-5</u>	<u>20173-24-4</u>	<u>20173-33-5</u>	<u>53295-70-8</u>	<u>71271-61-9</u>
	<u>76025-61-1</u>	<u>89850-73-7</u>	<u>89850-94-2</u>	<u>89910-55-4</u>	<u>90000-30-9</u>	<u>90197-12-9</u>
	<u>90203-22-8</u>	<u>90345-16-7</u>	<u>90434-63-2</u>	<u>90437-05-1</u>	<u>90482-84-1</u>	<u>90482-89-6</u>
	<u>90533-83-8</u>	<u>90533-86-1</u>	<u>90565-47-2</u>	<u>90565-48-3</u>	<u>90565-85-8</u>	<u>90796-47-7</u>
	<u>90872-84-7</u>	<u>90872-98-3</u>	<u>91010-50-3</u>	<u>91010-67-2</u>	<u>91010-98-9</u>	<u>91015-27-9</u>
	<u>91054-71-6</u>	<u>91054-72-7</u>	<u>91086-17-8</u>	<u>91086-18-9</u>	<u>91216-09-0</u>	<u>91429-75-3</u>
	<u>91429-93-5</u>	<u>91551-50-7</u>	<u>91551-54-1</u>	<u>91551-61-0</u>	<u>91688-26-5</u>	<u>91800-27-0</u>
	<u>91800-28-1</u>	<u>91800-29-2</u>	<u>91817-64-0</u>	<u>92033-42-6</u>	<u>92058-58-7</u>	<u>92058-67-8</u>
	<u>92255-17-9</u>	<u>92491-36-6</u>	<u>92492-76-7</u>	<u>92547-43-8</u>	<u>92869-96-0</u>	<u>93045-05-7</u>
	<u>93045-25-1</u>	<u>93045-26-2</u>	<u>93436-26-1</u>	<u>93761-79-6</u>	<u>94028-79-2</u>	<u>94866-37-2</u>
	<u>95742-86-2</u>	<u>95801-71-1</u>	<u>95809-58-8</u>	<u>96171-68-5</u>	<u>96172-77-9</u>	<u>100268-32-4</u>

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FILE 'REGISTRY' ENTERED AT 12:06:34 ON 24 MAY 2006

ANSWER 1 REGISTRY COPYRIGHT 2006 ACS on STN

RN 93947-69-4 REGISTRY  
 ED Entered STN: 30 Dec 1984  
 CN Pyridine, 3-[3-[(3,4-dimethoxyphenethyl)amino]propyl]- (7CI) (CA INDEX NAME)  
 FS 3D CONCORD  
 MF C18 H24 N2 O2  
 LC STN Files: CA, CAOLD, CAPLUS, CHEMCATS



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)  
 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

1 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

FILE 'CAOLD' ENTERED AT 12:06:35 ON 24 MAY 2006

=> fil reg; d acc 93045-25-1; fil CAOLD

FILE 'REGISTRY' ENTERED AT 12:06:39 ON 24 MAY 2006

ANSWER 1 REGISTRY COPYRIGHT 2006 ACS on STN

RN 93045-25-1 REGISTRY

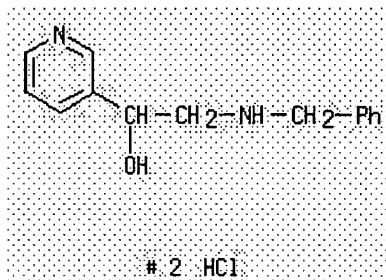
ED Entered STN: 18 Dec 1984

CN 3-Pyridinemethanol,  $\alpha$ -[(benzylamino)methyl]-, dihydrochloride (7CI)  
(CA INDEX NAME)

MF C14 H16 N2 O . 2 Cl H

LC STN Files: CA, CAOLD, CAPLUS

CRN (93045-26-2)



102 (b)

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

1 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

FILE 'CAOLD' ENTERED AT 12:06:39 ON 24 MAY 2006

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FILE 'REGISTRY' ENTERED AT 12:06:45 ON 24 MAY 2006

ANSWER 1 REGISTRY COPYRIGHT 2006 ACS on STN

RN 93045-26-2 REGISTRY

ED Entered STN: 18 Dec 1984

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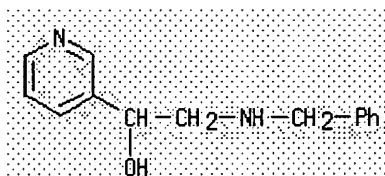
FS 3D CONCORD

MF C14 H16 N2 O

CI COM

LC STN Files: BEILSTEIN\*, CA, CAOLD, CAPLUS

(\*File contains numerically searchable property data)



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

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1 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

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